Tryptophan, methyl, 2-PFP

Inchi: InChI=1S/C17H10F10N2O4/c1-33-11(30)10(28-12(31)14(18,19)16(22,23)24)8-6-29(9-5-
InchiKey: AOAGFUVREFGYJI-UHFFFAOYSA-N
Formula: C17H10F10N2O4
SMILES: COC(=O)C(NC(=O)C(F)(F)C(F)(F)F)c1cn(C(=O)C(F)(F)C(F)(F)F)c2ccccc12
Mol. weight [g/mol]: 496.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.53		Crippen Method
logp	4.007		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
rinpol	1855.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580097&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices